
III.D.3 SOFC Modeling at PNNL

Objectives

- Develop and validate the multi-physics solid oxide fuel cell (SOFC) modeling tool to simulate the coupled SOFC stack performance.
- Utilize computational techniques for the mitigation of performance degradation and optimization of modular SOFC stack and systems design.
- Obtain necessary materials properties to support the development and optimization of SOFC designs through modeling.
- Disseminate/transfer modeling tool to all SECA industry teams and appropriate Core Technology Program (CTP) participants.

Accomplishments

- Implemented finite element SOFC electrochemistry module (SOFC-Multi Physics, SOFC-MP) fully compatible with the MARC finite element mesh and modeling capabilities to solve the coupled flow, electrochemistry, and heat transfer solution in the fuel cell under steady state conditions.
- Demonstrated a stack design tool for structural analysis from MSC Software called Mentat-FC, based on the SOFC-MP modeling capability for electrochemical, flow, and thermal analyses of SOFCs.
- Established a methodology to assess glass-ceramic seal failure and developed a continuum damage mechanics model based on the experimental stress/strain response for G18 sealing glass. The damage model was implemented in MSC MARC and was used for SOFC stack stress analysis to predict accumulated damage and failure of the seals under thermal-mechanical loading.

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- Conducted a comprehensive training program covering the full suite of SOFC modeling tools at the SECA Modeling Workshop.
- Developed a probabilistic-based component design methodology for SOFC stacks. This method takes into account the randomness in SOFC material properties as well as stresses arising from different manufacturing and operating conditions.
- Developed an integrated modeling/experimental framework to predict the life of SOFC interconnect materials. The effects of interconnect oxide growth on its structural integrity upon isothermal cooling have been studied using finite element analyses.

Introduction

In order to efficiently develop and optimize planar SOFC stacks, it is desirable to experiment numerically with the effects of stack component mass, geometry, flow rates of the gaseous reactants, electrical loading, and simulated aging. The computation of representative baseline cases, validated by experimental data, has been used to develop better understanding of the stack behavior while avoiding costly and time-consuming experiments. In order to model the multi-physics associated with an SOFC stack, a simulation tool, SOFC-MP was developed. This modeling tool combines the versatility of a commercial multi-physics code and a validated electrochemistry calculation routine. Its function is to predict the flow and distribution of anode and cathode gases, temperature and current distributions, and fuel utilization. The fundamental building blocks of modeling and simulation tools are electrochemical models, fluid flow simulations, computational mechanics and experimental data.

The multi-physics modeling tools developed were then used in studying the full range of design criteria as well as in material development and degradation modeling. On the stack level, a probabilistic-based component design methodology was developed. This method takes into account the randomness in SOFC material properties as well as stresses arising from different manufacturing and operating conditions. For SOFC materials development and degradation study, different degradation mechanisms for different SOFC components, i.e., seal and interconnect, have been considered in order to predict the useful operating time for the stack. Detailed seal and interconnect degradation mechanisms have been modeled and their influences on stack performance have been quantified.

Approach

- Maintain and enhance the integrated modeling tools developed under the SECA core program for evaluating fuel cell stack design concepts by the industrial teams.
- Investigate the effects of materials degradation on cell performance and cell life.
- Investigate the effects of cell geometric design, material property distributions and operating condition on SOFC reliability.

Results

Coarse Methodology – Finite Element Approach

An evaluation of the Mentat-FC and SOFC-MP modeling procedure was performed by studying temperature and stress predictions for a realistic planar design. The objective was to compare the predicted results from the highly efficient finite element model (generated with the Mentat-FC parametric graphical user interface (GUI) and solved by the SOFC-MP solver) with pre-existing results from a highly detailed but computationally expensive computational fluid dynamics (CFD) model. Results from the CFD model were available for an anode-supported planar cross-flow model with six fuel and air inlets/outlets. These results consisted of three cases that modeled i) pre-reformed fuel, ii) fuel with methane content for on-cell reformation, and iii) on-cell reformation using a lower activation energy to simulate a reduced reaction rate. The cell design and the operating conditions were replicated using the parametric build option in the Mentat-FC GUI to construct a highly similar geometry. There were minor features that differed between the two models (e.g. rounded outer corners, bolt holes), but all the essential geometric features of sizes, thicknesses, heights, and flow areas and all the operating conditions for fuel composition, inlet temperatures, velocities, and electrochemistry options were identical. The resulting temperature and stress distributions were presented and compared (Figure 1). In general, the temperature predictions were well matched for the geometry both qualitatively and quantitatively. Differences in the peak temperatures were noted and thermal distributions on the stack exterior were slightly different.

Coarse Methodology – Design Sensitivity Study

A probabilistic-based component design methodology has been developed for SOFC stacks. This method takes into account the randomness in SOFC material properties as well as stresses arising from different manufacturing and operating conditions. The purpose of this work is to provide the SOFC designers a 'coarse' design methodology such that the desired

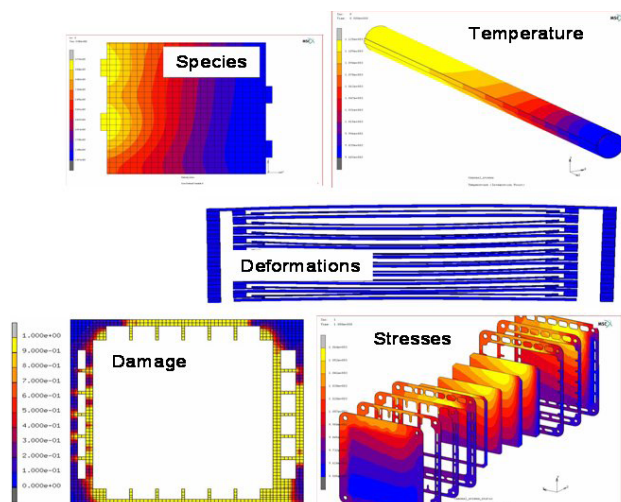


FIGURE 1. Typical SOFC-MP Modeling Results

level of component reliability can be achieved with deterministic design functions using an equivalent safety factor to account for the uncertainties in material properties and structural stresses. Component failure probabilities for the current design were then calculated under different operating conditions.

Seal Property Measurement, Prediction and Degradation Modeling

The glass-ceramic sealant G18 was expected to exhibit stress relaxation at elevated temperatures due to the viscoelastic response of the residual glass content. This would be important to include in SOFC stress analyses to better capture the stress state of the stack components. The continuum damage mechanics model for the glass-ceramic material developed previously was extended to include a viscoelastic response at high temperatures. A Maxwell-type model was used to capture the stress relaxation and used viscosities for the G18 material experimentally obtained at temperatures of 700-800°C (Figure 2). The response of the material model was demonstrated to capture the effect of viscosity and loading strain rate. The model was demonstrated in a single cell stack and compared to results using the previous elastic damage model (Figure 3). The stress relaxation made the cell more compliant and showed beneficial relaxation of the anode stresses through two thermal cycles.

Interconnect Degradation and Spallation Study

The effects of various oxide scale thickness on bulk and interface stresses are predicted for the ferritic stainless steel interconnect material, Crofer 22 APU, under isothermal cooling condition and micro-indentation. The goal of the study is to utilize the

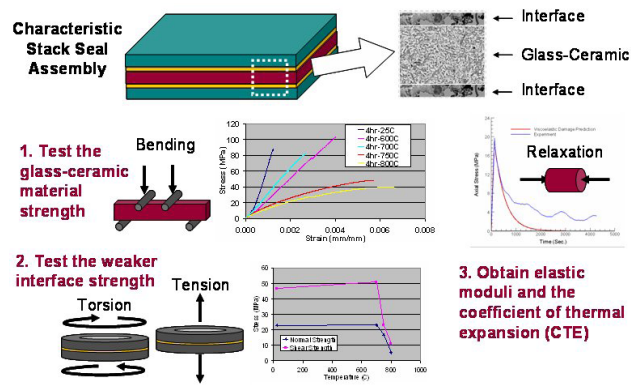


FIGURE 2. Seal Property Characterization

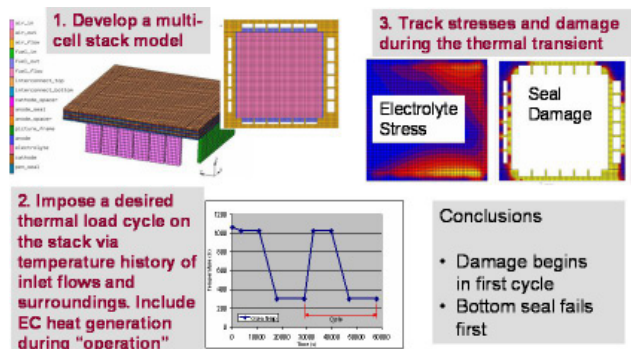


FIGURE 3. Seal Damage Modeling

measurement methodology and the associated quantified interfacial strength developed by other SECA team members in predicting possible scale spallation for different scale thickness, therefore indicating the possible interconnect life under isothermal cooling conditions (Figure 4).

Conclusions and Future Directions

- Continue to validate the model and to transfer the modeling tools technology to the SECA industry teams and work with them to increase utilization of the tools.
- Continue to add improved material models and numerical procedures to the modeling tools.
- Quantify bond strength of oxide/substrate for ferritic stainless steel to predict interconnect life under normal operating temperatures.
- Evaluate creep of glass-ceramic seals during thermal cycling operations.
- Develop seal property predictions via homogenization methods to identify desirable composite seal structures for stacks.

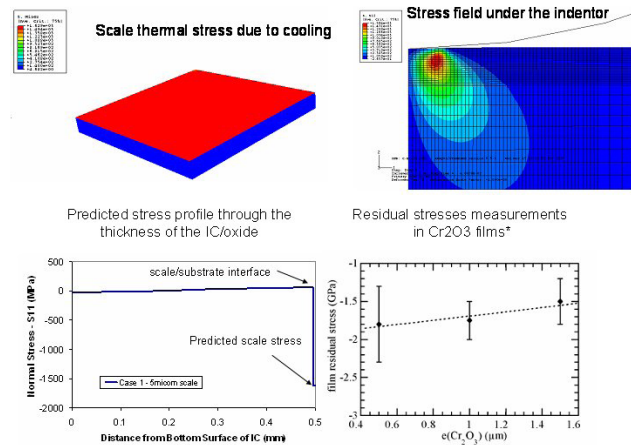


FIGURE 4. Interconnect Degradation and Life Modeling

- Develop analytical methods to evaluate the time-dependent mechanical behavior (creep, thermal fatigue, loss of interconnect contact) of fuel cell stacks/components and influence on electrochemical performance.

FY 2006 Publications/Presentations

1. "Effects of Oxide Thickness on Scale and Interface Stresses under Isothermal Cooling and Micro-Indentation", X. Sun, W.N. Liu, P. Singh and M.A. Khaleel, SECA Topical Report.
2. "Analysis of Seal Damage During Thermal Cycling of a Multi-Cell SOFC Stack", B.J. Koeppel, B.N. Nguyen, and M.A. Khaleel, SECA Topical Report.
3. "Experimental Characterization, Model Development, and Numerical Analysis of Glass-Ceramic Sealant Relaxation Under Thermal-Mechanical Loading", B.J. Koeppel, B.N. Nguyen, J.S. Vetrano, and M.A. Khaleel, SECA Topical Report.
4. "Mechanical Testing of Glass Seals for Solid Oxide Fuel Cells", J.S. Vetrano, Y.-S. Chou, G.J. Grant, B.J. Koeppel, B.N. Nguyen, and M.A. Khaleel, SECA Topical Report.
5. "Crack Growth in Solid Oxide Fuel Cell Materials: From Discrete to Continuum Damage Modeling", B.N. Nguyen, B.J. Koeppel, S. Ahzi, M.A. Khaleel and P. Singh, J. Am. Ceram. Soc. 89 [4] 1358–1368 (2006).
6. "On the Nonlinear Behavior of Glass-Ceramic Seal and Its Application in Planar SOFC Systems", B.N. Nguyen, B.J. Koeppel, J.S. Vetrano and M.A. Khaleel, Proceedings of FUELCELL2006 The 4th International Conference on Fuel Cell Science, Engineering and Technology June 19-21, 2006, Irvine, CA, FUELCELL2006-97057.
7. "Mechanical Property Characterizations and Performance Modeling of SOFC Seals", B.J. Koeppel, J.S. Vetrano, B.N. Nguyen, X. Sun, and M.A. Khaleel, 30th International Conference on Advanced Ceramics, Cocoa Beach, FL, January 23-27, 2006.

8. "Modeling and Measurement of Materials Behavior in Solid Oxide Fuel Cells", J. S. Vetrano, Y-S. Chou, B. Koepfel, B. Nguyen, M. Khaleel, Fuel Cell Seminar 2005, Palm Springs, CA.
9. "Multi-Component-Based Reliability Design for SOFC – A Coarse Design Methodology", X. Sun, A. Tartakovsky and M.A. Khaleel, Fuel Cell Seminar 2005, Palm Springs, CA.
10. Recent Development of Modeling Activities at PNNL, M.A. Khaleel, K.P. Recknagle, J.S. Vetrano, X. Sun, B.J. Koepfel, K.I. Johnson, V.N. Korolev, B.N. Nguyen, A.M. Tartakovsky, and P. Singh, SECA Core Technology Program Peer Review, Lakewood, CO, October 25-26, 2005.